Interaction of discrete breathers with electrons in nonlinear lattices

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ABSTRACT

We study the effects of electron-lattice interaction in the presence of discrete breathers. The lattice is treated classically. We consider two different situations - i) the scattering of an electron by a discrete breather in the semiconducting regime, where the electron-breather distance is large compared to the breather size, and ii) the appearance of a bound electron-breather state, which exists at least over one half of the breather period of oscillation. In the second case the localization length of the electron can be of the order of the breather size - a few lattice periods. Remarkably these results are derived in the absence of disorder, since discrete breathers exist in translationally invariant nonlinear lattices,

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I. INTRODUCTION

The concept of discrete breathers has been studied in detail in a number of publications [1], [2], [3], [4], [5], [6], [7], [8]. Discrete breathers are time-periodic solutions of a system of coupled classical degrees of freedom, typically arranged on a translationally invariant lattice. These solutions are spatially localized (note that spatial localization appears in the absence of any disorder). The number of degrees of freedom can be finite or infinite. A necessary condition for the appearance of discrete breathers is the presence of nonlinear terms in the equations of motion. A discrete breather can be viewed as a localized excitation of the system above its classical ground state. Localization occurs because multiples of the frequency of the breather can easily escape from resonances with the spectrum of the linearized equations of motion (around the ground state). This happens because the linear spectrum of the system (e.g. the phonon spectrum of a crystal) has a finite upper bound due to the discrete translational invariance (as opposed to a system with a continuous translational invariance, e.g. a field equation). Note that no specific topological requirements have to be met in order to obtain breather solutions, especially there are no restrictions with respect to the dimension of the lattice.

Although the concept of discrete breathers goes much beyond the description of nonlinear lattice dynamics in crystals, we will focus our attention in this work to crystals only. In particular we will study the problem of interaction of a discrete breather with electronic degrees of freedom. We will consider systems where screening effects due to mobile electrons are weak. In section II we derive the scattering of an electron by a discrete breather in the limit of large electron-breather distance. In section III the trapping of an electron by a discrete breather is analyzed. Remarkably the corresponding localization length of the electron can be of the order of the breather size, i.e. a few lattice sites.

II. SCATTERING OF AN ELECTRON BY A DISCRETE BREATHER

Let us consider a classical nonlinear lattice which allows for breather solutions. Generally the excitation of the relevant breather degrees of freedom leads to a localized polarization of the lattice. In the classical ground state of this system the polarization vanishes. If we excite a discrete breather, then it will induce a (time-periodic) multipole field at distances large compared to the breather size. Generally the first nonvanishing momentum will be a dipole momentum. The induced polarization will be spatially localized, in accord with the strong localization properties of the breather solution.

Let us consider the interaction of a single electron with a discrete breather in the case when the distance between the electron and the breather is much larger than the breather size. Since we are describing the lattice degrees of freedom classically, we can use the adiabatic approximation [9]. This means, that the motion of the electron is described by using the positions of the lattice degrees of freedom as parameters. Thus the electron feels a multipole field which originates from the breather. This kind of treatment of the electron is similar to the consideration of electrons in a lattice with defects [10]. The difference is, that i) the breather (dynamical defect) does not posess a uncompensated charge and ii) the breather is slowly (as compared to the inverse electron frequency) changing its multipole field.

Since the multipole field of the breather contains in general a dipole component, we can study the scattering of an electron in a dipole field. We consider the case when the electron can follow a path which does not come close to the breather location. If this assumption is not true anymore, the electron can be trapped by the breather, as will be shown in the next section.

The potential of a dipole is given by

$$V_d(\vec{r}) = \frac{1}{\epsilon} \frac{\vec{d}\,\vec{r}}{r^3} \quad . \tag{2.1}$$

Here $\vec{d}$ is the dipole moment induced by the breather (which is actually slowly periodically

oscillating with time). The dielectric permeability ϵ describes the reduction of the dipole field due to polarization effects.

The motion of an electron with isotropic effective mass m^* and charge e will be then described by the Hamiltonian H and the wave function $\Psi(\vec{r}, t)$ [10]

$$H = -\frac{\hbar^2}{2m^*}\Delta + eV_d(\vec{r}) \ , \ \ i\hbar\frac{\partial\Psi}{\partial t} = H\Psi \ . \tag{2.2}$$

The dipole potential (2.1) does not posess localized states. This can be easily found by considering the corresponding classical motion in the potential (2.1). Clearly there exist no periodic orbits having some finite distance from the potential center $\vec{r} = 0$. Thus there appear no localized electron states which are weakly localized as compared to the breather size. This situation is opposite to the Coulomb field problem where periodic orbits exist and lead to the existence of hydrogen like localized states, as used in the description of Wannier excitons. To find trapped electronic states induced by a discrete breather we have to take into account the internal breather structure, which will be studied in the next section.

To account for the elastic electron reflection in the dipole potential (2.1) we can use Born's approximation [9], which holds if the interaction energy between the electron and the breather will be small compared to the kinetic energy of the electron. Denoting by $|\vec{k}>$ the plane wave states of the electron in the absence of a breather, we have to calculate the matrix elements

$$<\vec{k}|V_d|\vec{k}'> = \int e^{i(\vec{k}-\vec{k}')\vec{r}}V_d(\vec{r})\mathrm{d}r^3 \ . \tag{2.3}$$

Straight integration gives

$$<\vec{k}|V_d|\vec{k}'> = -i\frac{4e\pi}{\epsilon}\frac{\vec{d}(\vec{k}-\vec{k}')}{|\vec{k}-\vec{k}'|^2}\delta(E_{\vec{k}} - E_{\vec{k}'}) \ . \tag{2.4}$$

The electronic energies $E_{\vec{k}}$ measure the energy of the incoming and outgoing plane waves. All other quantities related to the electron scattering in the used approximation can be obtained from these matrix elements.

In the nongeneric symmetric case that the breather does not posess a dipole momentum, the quadrupole field tensor $D_{\alpha\beta}$ has to be considered (note that we use the definition $D_{\alpha\beta} = \sum_i e_i x_\alpha^{(i)} x_\beta^{(i)}$). The corresponding potential is given by

$$V_q(\vec{r}) = \frac{1}{2\epsilon} D_{\alpha\beta} \frac{\partial}{\partial x_\alpha} \frac{\partial}{\partial x_\beta} \frac{1}{r} \quad . \tag{2.5}$$

Again there are no bound states in potential (2.5) as in the dipole case. The matrix elements can be obtained by integrating:

$$< \vec{k}|V_q|\vec{k'} > = -i \frac{2e\pi}{\epsilon} \frac{D_{\alpha\beta} k_\alpha k_\beta}{|\vec{k} - \vec{k'}|^2} \delta(E_{\vec{k}} - E_{\vec{k'}}) \quad . \tag{2.6}$$

Let us comment on possible numerical and experimental verifications of the results from this section. Numerical investigations can be performed if the motion of the electron is described within a tight-binding representation (cf. next section). For one-dimensional systems the task amounts to launching an electron wave with given wave number and accounting for its collision with a breather. The dependence of the transmission coefficient on the wave number can be then compared with our results. Similar studies were done for the scattering of phonons by breathers [11]. A numerical analysis of the two-dimensional case is also possible along the same lines, although it will be much harder and tedious. As for experiments, up to now there is no substantial knowledge on how to excite breathers, and how to provide a statistical description of scattering processes in the presence of breathers. Once the new collision integral [12] is obtained, one can think of possible experimental realizations to check the influence of breathers on the electrical conductivity.

III. TRAPPING OF AN ELECTRON BY A DISCRETE BREATHER

In this section we analyze the properties of localized electronic states, induced by the presence of a discrete breather. We restrict the consideration to the simplest case of a one-dimensional tight-binding description of the electron [13], where the overlap integral of the electron states at neighbouring sites depends on the positions of the corresponding crystal atoms.

Again we describe the crystal atoms classically, so that we have to use the adiabatic approximation. Consequently we can treat only electronic states, which are energetically well separated from other electronic states. An electron sitting in such an adiabatic state will continue to stay in this state if the Hamiltonian of the electron is changed adiabatically slowly (due to the motion of the crystal atoms). Clearly we can not consider extended electronic states, which usually form a band (so that the energy separation is violated). The idea is then to show that at some intervals in time the localized lattice distortion due to the presence of a discrete breather allows for localized electronic states, which are well separated from the electronic band. If an electron is occupying such a localized state, the dynamics of the breather will be changed according to the adiabatic approximation.

The Hamiltonian H of the system is given by

$$H_{lat} = \sum_l \left[\frac{1}{2}P_l^2 + V(X_l) + \Phi(X_l - X_{l-1}) \right] \ , \tag{3.1}$$

$$H_{el} = \sum_l \beta_{l,l+1}(a_l^+ a_{l+1} + cc) \ , \ \ \beta_{l,l+1} = 1 + \beta_1(X_l - X_{l-1}) \ , \tag{3.2}$$

$$H = H_{lat} + H_{el} \ . \tag{3.3}$$

The lattice part H_{lat} contains anharmonic terms ($\partial^2 H_{lat}/\partial X_l \partial X_{l'} \neq$ const) in the potential functions $V(z)$ and $\Phi(z)$. The electron-lattice coupling is considered in linear approximation in the overlap integral β. The one-site electronic energies are assumed to be independent on the lattice site number l, so that the corresponding terms $a_l^+ a_l$ can be scaled away in (3.2).

The adiabatic approximation implies to solve the eigenvalue problem for the electron (3.2) using the lattice degrees of freedom as fixed parameters. The electronic band for (3.2) is given by

$$E_k = 2\cos(k) \tag{3.4}$$

(here k measures the wavenumber of the extended electron wave).

To account for the localized state of the electron in the presence of a discrete breather we arrive at the equations for the probability amplitudes c_l of finding the electron at lattice site l:

$$E_{el}c_l = \beta_{(l-1),l}c_{l-1} + \beta_{l,(l+1)}c_{l+1} \ . \tag{3.5}$$

In order to proceed we have to use a known discrete breather solution. It is known that breather solutions exist, when essentially one (central) atom is performing periodic oscillations, with all the other atoms having exponentially small amplitudes [6], [8], [14]. Discrete breathers with such strong localization properties were found in numerical studies for one-dimensional and two-dimensional lattices with moderate coupling and anharmonicity [4], [5]. Thus we assume the easiest form of the breather solution to be, that only one central particle is oscillating (with a frequency outside the linear phonon spectrum). Taking into account the small (compared to the central atom) amplitudes of vibration of the rest of the lattice leads to small corrections of the results derived below.

If the breather is essentially given by the motion of one atom $X_0(t) = X_0(t + T_b)$, then we can solve analytically for the electronic state. All other atoms are at their groundstate positions $X_{l\neq0} = 0$. Solving (3.5) to the left and right of the breather location yields

$$c_l = c_1 e^{-\lambda l} \ , \quad l > 1 \tag{3.6}$$

$$c_l = c_{-1} e^{\lambda l} \ , \quad l < -1 \tag{3.7}$$

$$E_{el} = 2\cosh(\lambda) \ . \tag{3.8}$$

To obtain the energy E_{el} we have to match the two branches of our solution in the breather center, when the amplitude of the central atom at a given time is $X_0(t)$. The result is

$$E_{el} = \frac{1}{\sqrt{1 + 2\beta_1^2 X_0^2(t)}} + \sqrt{1 + 2\beta_1^2 X_0^2(t)} \approx 2 + \beta_1^4 X_0^4(t) + O(\beta_1^6 X_0^6(t)) \ . \tag{3.9}$$

The exponent of the spatial decay of the electronic localized state λ is then given by

$$\lambda = \frac{1}{2}\ln(1 + 2\beta_1^2 X_0^2(t)) \ . \tag{3.10}$$

The unnormalized probability amplitudes in the center of the breather location are given by

$$c_0 = 1 \ , \tag{3.11}$$

$$c_1 = \sqrt{1 + 2\beta_1^2 X_0^2(t)}(1 - \beta_1 X_0(t)) \ , \tag{3.12}$$

$$c_{-1} = \sqrt{1 + 2\beta_1^2 X_0^2(t)}(1 + \beta_1 X_0(t)) \ , \tag{3.13}$$

The dynamics of the discrete breather is now modified due to the additional purely anharmonic electron-induced potential (3.9). Depending on the breather solution (frequency above or below the phonon band) this additional potential can either support the localized breather solution or supress it [14]. Remarkably there *is* a realization when it can support the breather solution - that means that the breather gets even more strongly localized, inducing again a more strong localization of the electronic state etc.

It is worthwhile to mention a numerical study, where the lattice itself does not support discrete breathers, but a bound electron-breather state exists [15], [16]. We can give a simple explanation to this observation. The relevant expansion parameters for the potential $\Phi(z) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} \phi_\mu (z - z_0)^\mu$ in [15], [16] are given by $\phi_2 = 0.005625$, $\phi_3 = -0.004922$, $\phi_4 = 0.001812$. It has been shown recently, that breather solutions do not exist for that lattice, because the inequality $3/4 \phi_2 \phi_4 \geq \phi_3^2$ is not fulfilled. This steems from the fact, that the corresponding upper zone boundary plane wave undergoes a tangential bifurcation only if the above inequality *is* fulfilled [17], [18]. However the correction of the lattice potential energy due to a (initially) localized electron can change this relation locally (cf. (3.9)), so that breathers can exist if a localized electronic state is occupied.

Since $X_0(t)$ of the breather solution becomes periodically zero, the adiabatic approximation will become invalid every half-period of the breather's oscillation. That happens because the localized state of the electron merges with the electron band states. So we conjecture that a trapped (localized) electronic state may exist only over roughly every half-period of the breather. That observation follows from the circumstance that the adiabatic approximation holds if the separation of the localized state from the continuum is much larger than the change of interaction energy during one period of the electronic amplitude oscillations which implies

$$\beta_1^4 X_0^5(t) \gg \dot{X}_0(t) \ .$$

Each time when the central atom will pass its stability position $X_0 = 0$ the localized electronic state will come close to the electronic band. Consequently some part of the initially

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localized electron wave function will be emitted into the electronic band. This will lead to a finite life time of the localized electronic state of the order of one half of the breather period (this can be also seen in the numerical result in [15], [16]).

We also briefly mention the case of another breather symmetry, when a breather is given essentially by the motion of two nearest neighbours $X_0(t) = -X_1(t)$. These two-site breathers appear with frequencies above the linear spectrum (phonon band). Relations (3.6)-(3.8) hold again. The energy of the localized electronic state is given by

$$E_{el} = F + \frac{1}{F} \quad , \tag{3.14}$$

$$F = \frac{2x + 1 - \sqrt{1 + 8x^2 - 4x}}{2x(2 - x)} \quad , \quad x = \beta_1 X_0(t) \quad . \tag{3.15}$$

Note that in lowest order of $\beta_1 X_0(t)$ the energy again becomes

$$E_{el} \approx 2 + \beta_1^4 X_0^4(t) + O(\beta_1^5 X_0^5(t)) \quad . \tag{3.16}$$

Here we have considered highly discrete (localized) breather solutions only. Taking into account the (nonzero) oscillations of the other atoms in the breather solution will smoothly modify our findings, but can not change them qualitatively (unless the breather becomes very weakly localized).

Let us consider the case of higher dimensional lattices. Discrete breathers can be obtained in full analogy to the one-dimensional case. However the localization properties of the electron will be modifed. In two-dimensional lattices the separation of the localized electronic state from the electronic band will be exponentially small for small breather amplitudes [19]. In three-dimensional lattices the discrete breather amplitude has even to exceed a certain finite threshold in order to localize an electron [19]. So in higher dimensional lattices the trapping time of an electron will be shortened as compared to the one-dimensional case.

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